Supplemental Material

First Principles Predicting Enhanced Ductility of Boride Carbide through Magnesium Microalloying

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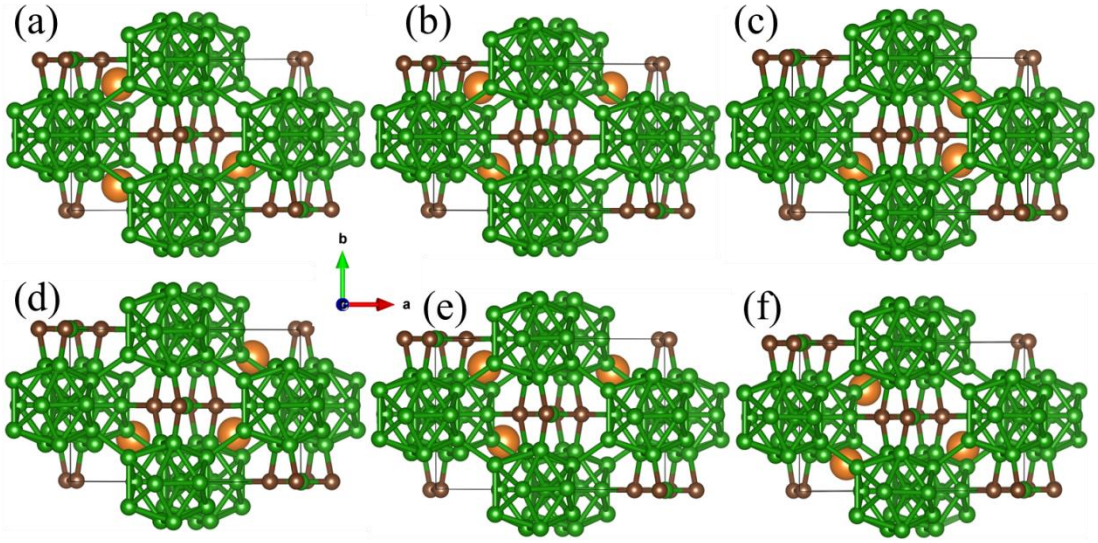

Fig. S1. Six possible structures for $Mg_3B_{50}C_8$ based on various occupation sites for Mg atoms. (a) Mg partial occupation sites is Mg1-Mg2Mg1; (b) Mg partial occupation sites is Mg1-Mg1Mg2; (c) Mg partial occupation sites is Mg1-Mg2Mg2;(d) Mg partial occupation sites is Mg2-Mg1Mg1; (e) Mg partial occupation sites is Mg2-Mg1Mg2; (f) Mg partial occupation sites is Mg2-Mg2Mg1.

Table S1. The possible atomic structures from Mg partial occupation and electronic energies (unit eV). + represents that the structure is relaxed to a stable structure after structural optimization. The Mg1 and Mg2 positions are shown in Fig. 1(b).

Possible atomic structure	Electronic energy (eV)	Relative energy (eV)
Mg1-Mg2Mg1	-421.360	0
Mg1-Mg1Mg2	-421.360	0
$^{+}$Mg1-Mg2Mg2	-421.359	0.001
$^{+}$Mg2-Mg1Mg1	-421.359	0.001
Mg2-Mg1Mg2	-421.359	0.001
Mg2-Mg2Mg1	-421.360	0

Table S2. DFT Predicted Elastic Modulus for $Mg_3B_{50}C_8$ (unit kbar)

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	4208.8	831.2	651.0	128.0	-9.8	-155.0
YY	831.2	5460.0	817.8	58.3	1.7	134.4
ZZ	651.0	817.8	5295.3	19.7	-2.7	138.4
XY	128.0	58.3	19.7	1639. 7	173.8	4.7
YZ	-9.8	1.7	-2.7	173.8	2207.6	59.5
ZX	-155.0	134.4	138.4	4.7	59.5	1416.8